Polarization of interacting bosons with spin

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We prove that in the absence of explicit spin-dependent forces one of the ground states of interacting bosons with spin is always fully polarized. Generally, this state is degenerate with other states, but one can specify the exact degeneracy. For $T > 0$ the magnetization and zero-field susceptibility exceed that of a pure paramagnet. The results are relevant to experimental work on triplet superconductivity and condensation of atoms with spin. They eliminate the possibility, raised in some theoretical speculations, that the ground state or positive temperature state might be antiferromagnetic.

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Bosons with spin first appeared in condensed matter physics in the theory of ^{3}He superfluidity, which is due to spin-triplet p-wave pairing of the Helium atoms [1]. More recently they were discussed in connection with the rising interest in triplet superconductivity [2, 3, 4, 5] and multicomponent Bose-Einstein condensation [6, 7, 8]. The renewed fascination with spin-triplet superconductivity was generated by recent experimental evidence for triplet pairing in heavy fermion systems [2], organic conductors [3], and the layered oxide Sr_2RuO_4 [4, 5]. Recent advances in the study of the Bose-Einstein condensation phenomenon enabled condensation of bosons with nonzero spin (spin-1 in particular), such as ^{23}Na and ^{87}Rb atoms, by confining them in optical traps rather than the usual magnetic traps, thus preserving their spinor nature [6, 7].

Moreover, it is possible to have condensates of bosons with other internal degrees of freedom which behave like spin, thus realizing "spin-1/2" bosons. For example, a two component Bose gas was produced in a magnetically trapped ^{87}Rb condensate by rotating two hyperfine states into each other, creating an $SU(2)$ symmetry [8].

All these experimental achievements have generated new interest in the study of interacting spinor bosons. In particular, some tantalizing hints for a possible connection between the onset of triplet superconductivity and the appearance of internal magnetic moments [4] call for better understanding of the magnetic properties of strongly interacting bosons. We report here an exact and general result, stating that for a generic Hamiltonian of bosons with spin, a fully polarized state is among the ground states – as long as there are no explicit spin-dependent forces – however complicated the many-body interaction potential might be. We can also classify all other ground states. The conclusion is that the ground state susceptibility is infinite. We further show that the positive temperature magnetization and zero-field susceptibility exceed those of non-interacting distinguishable (Maxwell-Boltzmann) spins.

Recent works [9] analyzed the two body interaction for spin-1 atoms in an optical trap. Using an effective low energy approach, the interaction term was parameterized there by

$$V(\mathbf{r}_i - \mathbf{r}_j) = \delta(\mathbf{r}_i - \mathbf{r}_j)(c_0 + c_2 \mathbf{S}_1 \cdot \mathbf{S}_2) \qquad (1)$$

where the coefficients c_0 and c_2 are related to the s-wave scattering lengths in the singlet and triplet channels. The possibility of an antiferromagnetic coupling $c_2 > 0$ has attracted much attention in the past few years. Experimental estimates for these scattering lengths suggest that $c_2 > 0$ for a condensate of ^{23}Na atoms [10]. In such a case, the energy is minimized by a polar state with $\langle \mathbf{S} \rangle = 0$. We point out that in view of the following exact results this scenario can be ruled out as long as the full many-body interaction is spin-independent. In fact, as we explain later, the theorem below shows that the effective two-body spin-dependent interaction described in Eq. (1) can not describe the low-energy behavior of bosons with spin-independent interaction, *no matter what the sign of* c_2 *is.* Therefore, a bosonic spin-spin term of the type (1) can only be justified by going beyond a spin-independent bosonic Hamiltonian, either by introducing explicit spin-dependent forces, or by taking into account the underlying fermionic physics of the atoms. This situation should be contrasted with the fermionic case in which effective exchange interactions, ferromagnetic or antiferromagnetic, do come about from spin-independent Hamiltonians.

The Hamiltonian of a Bose gas of N bosons, and without spin-dependent forces, is given by

$$H = -\sum_{i=1}^{N} \frac{1}{2m} \nabla_i^2 + v(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N) \qquad (2)$$

where m is the mass of the bosons, and $\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N$ are the spatial coordinates of the bosons. v is a spin-independent, totally symmetric, potential, which includes any confinement, disorder, and k-body interactions. We look for the lowest energy state that is totally symmetric under permutations of the space-spin indices.

To find it, we temporarily ignore both the spin of the particles and the identity of the bosons at first, and look for the ground state of N *non-identical particles*, i.e., particles without spin and without any symmetry restriction on the wave-function. We seek the absolutely lowest state of H, $\psi(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N)$.

It is known (e.g., [11]) that this ground state is unique (up to an overall phase) and satisfies

$$\psi(\mathbf{x}_1, \cdots, \mathbf{x}_N) > 0 \qquad \text{for all} \;\; \mathbf{x}_1, \cdots, \mathbf{x}_N \tag{3}$$

(unless v is so repulsive that it prevents particles from changing places by a continuous path – which would be non-physical). This result holds for all boundary conditions (Dirichlet, von-Neumann, periodic). Eq. (3) follows immediately from the fact that ψ can be chosen to be real (because ψ^* is also a ground state and hence $\psi \pm \psi^*$ are ground states), and from the fact that the variational energy of the function $|\psi|$ then equals that of ψ itself [12, Eq. (6.17.2)]. Hence $|\psi|$ must be a ground state. From this we conclude that if ψ is a real ground state, either $\psi = \alpha|\psi|$, and thus (3) is satisfied, or $|\psi| - \psi$ is a ground state that is zero on a set of positive measure, which is impossible unless v has the pathology mentioned above. If, now, ϕ is another real ground state that is orthogonal to ψ then $\phi = |\phi|$ up to a phase (as we just proved). But two positive functions cannot be orthogonal, so ψ is unique.

Equation (3) implies that ψ must be totally symmetric. I.e., if we sum ψ over all permutations we obtain a function that is (a) symmetric, (b) non-zero, and (c) a ground state. By uniqueness, this symmetric function must equal ψ up to a constant.

We now return to our identical spin-full boson problem, and define

$$\phi(\mathbf{x}_1, \cdots, \mathbf{x}_N; \sigma_1, \cdots, \sigma_N) \equiv \psi(\mathbf{x}_1, \cdots, \mathbf{x}_N)| \uparrow\uparrow\uparrow \cdots\rangle$$

This function is totally symmetric in both spin and spatial indices, and thus is a valid wave-function for bosons (with spin). As we have shown it minimizes the energy regardless of symmetry restriction, and is, therefore, a ground state of the boson system.

This ground state has spin angular momentum $J = NS$, where S is each boson's spin, and carries the usual $(2SN + 1)$-fold degeneracy. There will be other ground states, but each must be a spin function times the unique spatial function we have just described. The question of the ground state degeneracy thus reduces to the following question: How many different spin functions are there that are totally symmetric (up to the trivial $2J + 1$-fold degeneracy)? The answer is as follows.

(i). If $S = 1/2$ ("spin-1/2" bosons [13]) then there is just one function, $J = N/2$, and the ground state is therefore non-degenerate (except for the trivial degeneracy).

(ii). If $S = 1$ there are functions with $J = N$, $N - 2$, $N - 4, \ldots$ and each of these appears exactly *once.* Wave-functions with $J = N - 1$, $N - 3$, $N - 5, \ldots$ do not appear in the ground state. This is contrary to what one would have for a paramagnet in which all J values are degenerate, and J-values smaller than N occur multiple times.

(iii). Other values of S can be similarly analyzed by studying representations of $SU(2S + 1)$ or by studying $(2S + 1)$-rowed Young's tableaux.

If a magnetic field term $H_M = -\mu h \sum_{i=1}^N \sigma_i^z$ (where h is the field, and $\mu\sigma_i^z$ is the atomic magnetic moment in the $\hat{z}$ direction, including the g-factor), is added to H then the ground state energy shifts by $-\mu hNS$, i.e., the zero-field susceptibility is infinite.

We now discuss the positive temperature case and compare it with pure paramagnetism. In the following, a pure paramagnet means a set of N non-interacting, distinguishable, spin-S particles, which has no degrees of freedom besides the spin. The pure paramagnet magnetization is, therefore,

$$\begin{aligned} M^{\rm para}(T,h) &= N\mu \, \frac{\sum_{\sigma=-S}^{S} \sigma \exp[\beta\mu h\sigma]}{\sum_{\sigma=-S}^{S} \exp[\beta\mu h\sigma]} \\ &= \frac{N\mu}{2} \left[(2S+1)\coth\left(\frac{2S+1}{2}\beta\mu h\right) \right. \\ &\qquad \left. - \coth\left(\frac{1}{2}\beta\mu h\right) \right], \end{aligned} \tag{4}$$

where $\beta = 1/k_BT$.

Our theorem about enhanced magnetization in the ground state can be generalized to positive temperature T, as follows.

THEOREM: *For each T and magnetic field $h > 0$, the magnetization $M(T, h)$ is greater than the pure paramagnetic value $M^{\rm para}(T, h)$. Moreover, the zero-field susceptibility $\partial M(T, h)/\partial h|_{h=0}$, also exceeds that of a pure paramagnet, $\partial M^{\rm para}(T, h)/\partial h|_{h=0}$.*

Proof.— Let us denote a particle configuration $x_1, x_2, ..., x_N$ by X and a spin configuration (in the σ^z basis) $\sigma_1, \sigma_2, ...\sigma_N$ by Σ. Since spin does not enter H except through H_M the (operator) Boltzmann factor has the kernel

$$K(X, X'; T) \exp\left[\, \beta\mu h S(\Sigma) \,\right] \delta_{\Sigma,\Sigma'}$$

where $S(\Sigma) = \sum_{i=1}^N \sigma_i^z$, $\delta_{\Sigma,\Sigma'}$ is the 'Kronecker delta' $\Pi_{i=1}^N \delta_{\sigma_i,\sigma_i'}$ and K is the (unsymmetrized) kernel of $\exp[\,-\beta H\,]$. The symmetrized Boltzmann factor is then

$$\mathcal{S}_{X,\Sigma}\, K(X, X'; T) \exp\left[\, \beta\mu h S(\Sigma) \,\right] \; \delta_{\Sigma,\Sigma'} \; . \tag{5}$$

and $\mathcal{S}_{X,\Sigma}$ is the symmetrizer on the X, Σ variables. (It is not necessary to symmetrize on the X', Σ' since this will be automatic.)

The important point to notice is the $T > 0$ analogue of (3), namely, $K(X, X'; T) > 0$ for all X, X' (outside of a 'hard-core' region). This can easily be seen by the

path-space (Wiener) integral for $\exp[-\beta H](X, X')$ via the Feynman-Kac formula – or else via the Trotter product formula [14].

The Trotter formula states that $\exp[-\beta H](X, X')$ is the limit as $N \to \infty$ of

$$\int A(X, X_1)B(X_1, X_2)A(X_2, X_3)B(X_3, X_4)\cdots A(X_{2N-2}, X_{2N-1})B(X_{2N-1}, X')dX_1\cdots dX_{2N-1} \quad (6)$$

where $A(X,Y) = \exp[-\beta H_0/N](X,Y)$ (with H_0 = kinetic energy operator) and $B(X,Y) = \exp[-\beta v/N](X,Y) = \exp[-\beta v(X)/N]\delta(X-Y)$. The kernel A is a Gaussian, $A(X,Y) = C_1 \exp[C_2(X-Y)^2]$. Since all kernels are nonnegative, we see that the multiple integral (6) yields a nonnegative function. The limit of nonnegative functions is nonnegative and, with some work one can show that $K(X, X'; T) > 0$ for all X, X' (outside of a 'hard-core' region). In case $\exp[-v(X)]$ is not integrable we must first approximate it by a bounded function and then remove the approximations at the end. The positivity of the kernel is conserved under symmetrization.

In fact, the only thing we really need is the weaker assertion that $K_\pi(X;T)$, defined below, is nonnegative and is positive on a set of positive X measure.

To calculate the partition function $Z(T,h)$ we set $X = X'$ and $\Sigma = \Sigma'$ (after applying $\mathcal{S}_{X,\Sigma}$) and then integrate over X and sum over Σ (i.e., $\sum_\Sigma = \Pi_{i=1}^N \sum_{\sigma_1=-S}^S$). We obtain an expression of the form

$$Z(T,h) = \frac{1}{N!}\sum_\pi \int dX K_\pi(X;T) \times \sum_\Sigma \exp\left[\beta\mu h S(\Sigma)\right]\delta_{\pi(\Sigma),\Sigma} \ ,$$

where the first summation is over all permutations π and $K_\pi(X;T)$ is a π-dependent function of X and T defined by $K_\pi(X;T) = K(\pi X,\ X;T)$.

To compute $M(T,h)$ let us define

$$Z_\pi(T,h) = \sum_\Sigma \exp\left[\beta\mu h S(\Sigma)\right]\delta_{\pi(\Sigma),\Sigma} \ , \quad (7)$$

$$M_\pi(T,h) = \frac{\sum_\Sigma S(\Sigma)\exp\left[\beta\mu h S(\Sigma)\right]\delta_{\pi(\Sigma),\Sigma}}{Z_\pi(T,h)} \ , \quad (8)$$

$$C_\pi(T,h) = Z_\pi(T,h)\int K_\pi(X;T)dX \ . \quad (9)$$

Then we can write

$$M(T,h) = \frac{\sum_\pi C_\pi(T,h)M_\pi(T,h)}{\sum_\pi C_\pi(T,h)} \ . \quad (10)$$

Since $K(X,X';T) \geq 0$ and > 0 on a set of positive X measure, $C_\pi(T,h) > 0$, and we have that $M(T,h) > \min_\pi\ M_\pi(T,h)$. (The strict inequality $>$ follows from the facts that $C_\pi(T,h) > 0$ and that the numbers $M_\pi(T,h)$ are not all equal.)

Our problem reduces to deciding which π will make (8) as small as possible. It is the identity permutation, and this gives $M^{\rm para}(T,h)$ as the lower bound. To see this we note that $M_\pi(T,h)$ is the magnetization of distinguishable particles that interact only through the constraint given by $\delta_{\pi(\Sigma),\Sigma}$. If π is the identity, there is no constraint, and one gets the pure paramagnetic magnetization (4). For any other permutation π, $\delta_{\pi(\Sigma),\Sigma}$ connects a group (or groups) of, say, $k > 1$ spins. There is one group of size k for each cycle of length k in π. This grouping only raises the magnetization by reducing the entropy of the low moment states. In other words, the assertion follows from the inequality

$$k\frac{\sum_{\sigma=-S}^S \sigma\exp[\beta\mu h\sigma]}{\sum_{\sigma=-S}^S \exp[\beta\mu h\sigma]} < \frac{\sum_{\sigma=-S}^S (k\sigma)\exp[\beta\mu h(k\sigma)]}{\sum_{\sigma=-S}^S \exp[\beta\mu h(k\sigma)]}$$

whose validity can be immediately seen by rewriting it as $kM(T,h) < kM(T/k,h)$. This inequality means that the magnetization of each group of k spins is higher than that of k independent spins. Since the magnetization of different groups is additive, we conclude that the constraint of tying together a group of spins increases the magnetization; therefore, the minimal $M_\pi(T,h)$ occurs at π being the identity.

Finally, the fact that the $h=0$ susceptibility exceeds the paramagnetic value follows from the two facts that $M(T,0) = 0$ and $M(T,h)$ is greater than the paramagnetic value for all h. Q.E.D.

Some Generalizations.—

(A) The previous results hold true even if there are several species of bosons in the system, with possibly different masses, as long as there are no fermions present. The only difference is that the degeneracy of the ground state is the product of the degeneracies found in (i), (ii), (iii) above for each species.

(B) The results hold for a 'relativistic' boson system obtained by replacing $p^2/2m$ by $\sqrt{p^2+m^2} = \sqrt{-\nabla^2+m^2}$. The underlying reason is that the kernel of $\exp\left[-\beta\sqrt{p^2+m^2}\right]$ is also positive [12, Eq. (7.11.11)]. Lest the reader think that positivity is a triviality, we remark that it does not hold for $\exp\left[-\beta p^4\right]$.

(C) Our results hold in any dimension, of course. They also hold in lattice models (e.g., sometimes called 'Bose-Hubbard' models) in which the Δ in the kinetic energy, $-\Delta = -\nabla^2$, is replaced by the discrete lattice Laplacian (= second difference operator) or $\sum_{\langle i,j\rangle} a_i^\dagger a_j$ in the usual second quantized notation. No regularity of the lattice is needed; indeed, the 'lattice' can be any general connected graph.

Several recent works have discussed boson models with an antiferromagnetic coupling in the effective low-energy

Hamiltonian, resulting in a polar ground state. Our theorem eliminates the possibility of the Hamiltonian (2) producing an antiferromagnetic state for bosons. Furthermore, it follows that the low energy parameterization (1) of the Hamiltonian (2) *must have* $c_2 = 0$. To be specific, we discuss the spin-1 case, but the situation is similar for bosons with higher spin. The potential (1) with $c_2 = 0$ satisfies the conditions of our theorem, and therefore its ground state for spin-1 bosons is degenerate, having states with $J = N$, $N-2$, $N-4$, ... Switching on the spin-spin interaction, with non-zero c_2, would choose between these degenerate states, break the degeneracy, and contradict the theorem. Therefore, a non-zero c_2 is inconsistent with a correct low energy theory of the Hamiltonian (2). Possible sources for such spin-spin interaction are then the (rather weak) direct dipole-dipole magnetic interaction, or exchange terms coming from the electron transfer between the atoms, thus going beyond the bosonic description of the system.

In a recent experiment [7] the magnetic structure of a Bose-Einstein condensate of spin-1 ^{87}Rb atoms was explored. The authors studied the distribution of the different magnetic number m values, but did not look at the global polarization properties. Based on the above, we suggest looking at the magnetization at finite field strength. According to the paramagnetic lower bound (4), the magnetization at the experimental temperature should exceed half of the maximal magnetic moment at fields as low as 1G. One can also rotate the macroscopic magnetic moment of the condensate to a specific direction (by an appropriate magnetic field), and then (after switching off the field and allowing for relaxation) measure the distribution of the m values, quantized along the same axis. A macroscopic moment should show up as a large fraction of the bosons in the $m = 1$ state. As discussed above, violation of the above predictions would indicate the importance of additional interaction terms, going beyond the Hamiltonian (2).

In conclusion, we have shown that fully polarized states are among the ground states of interacting bosons. Moreover, the finite temperature magnetization and zero-field susceptibility were shown to be bigger than that of Maxwell-Boltzmann (distinguishable) free spins. Our results hold in the presence of random on-site disorder and density-density interactions. They hold even if there is no interaction potential at all, because our theorems apply to the Hamiltonian $H = \sum p^2/2m$ as well. They might be relevant for recent experiments suggesting the formation of an internal magnetic moment at the onset of spin-triplet superconductivity, and to recent magnetic measurements of Bose-Einstein condensates. In particular, our ground state result constrains effective low-energy theories for interacting bosons, namely, it excludes the possibility of a spin-spin two-body term in the absence of explicit spin-dependent interactions in the underlying Hamiltonian.

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Note added in proof.– After this paper was submitted for publication we learned that similar mathematical results were obtained by András Sütő [15] in a study of "cycle percolation" in Bose gases. Our theorem that the pure paramagnetic value is a lower bound to the magnetization for nonzero field was not given there, however.

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